

# Cluster decomposition of percolation probability on the hexagonal lattice

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The upper estimate of the percolation threshold of the Bernoulli random field on the hexagonal lattice is found. It is done on the basis of the cluster decomposition. Each term of the decomposition is estimated using the number estimate of cycles on the hexagonal lattice which represent external borders of possible finite clusters containing the fixed lattice vertex.

**1. Introduction.** Generally, the percolation theory studies random subsets of the infinite set where the filtering relative to the inclusion and the supplementary connectedness relation has been defined [1]. In particular, such a theory may be arisen in noncompact topological space where filtering is defined by sequences of compact spaces when their union coincides with the total space [2]. The problem of existence of the random realization with connected noncompact components represents the main interest. In the case when the probability of such an event is positive, they say that the percolation is present in the random set. The calculation of the percolation probability represents the difficult mathematical problem even in most simple mathematical structures pointed out. Therefore, they resort usually to computer experiments for the problem solving when the percolation theory is applied and there are some considerable achievements in this direction (see, for example, [3]). In this work, we study the pointed out problem from the mathematical point of view. Usually, due to the extreme complexity of the problem, such investigations are connected with the study of elementary noncompact spaces such as integer lattices  $\mathbb{Z}^d$ ,  $d = 2, 3$  with the definite connectedness relation. The definition of this relation transforms integer lattices into those mathematical objects which are called periodic graphs [4]. Percolation on periodic graphs is the subject of *the discrete percolation theory*. However, even for periodic graphs, the main problem of percolation theory are resisted to mathematical processing only for random sets generated by the Bernoulli field  $\{\tilde{c}(\mathbf{x}); \mathbf{x} \in \mathbb{Z}^d\}$  when the probability distribution defined by the unique parameter  $c = \Pr\{\tilde{c}(\mathbf{x}) = 1\}$ . In this work, it is found the upper estimate of the so-called *percolation threshold*  $c_*$  in the case of the two-dimensional uniform periodic graph which is called the hexagonal lattice. The percolation probability  $Q(c)$  is differed from zero at  $c > c_*$ . Our estimate is done by the well-known approach which we name *the*

*cluster decomposition* (see also [5], [6]). To estimate the value  $c_*$ , we find the upper estimate of the number of finite clusters on the hexagonal lattice which contain the fixed lattice vertex.

**2. The percolation theory problem on the hexagonal lattice.** First of all, we introduce some geometrical objects modeling crystal lattices. After that we will set the problem of the discrete percolation theory on such mathematical structures. In connection with the purpose of the present work, we consider only two-dimensional lattices.

We name the infinite set  $V$  in  $\mathbb{R}^2$  the periodic one if there is the pair  $\langle \mathbf{e}_1, \mathbf{e}_2 \rangle$  of not collinear vectors in  $\mathbb{R}^2$  (the parallelogram of periods) such that the relation  $V = V + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2$  takes place for any  $n_i \in \mathbb{Z}, i \in \{1, 2\}$ . We name the periodic set in  $\mathbb{R}^2$  *the crystal lattice* if it consists of isolated points. The crystal lattice admits the disjunctive decomposition  $V = \bigcup_{\langle n_1, n_2 \rangle \in \mathbb{Z}^2} \{V_0 + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2\}$

where the finite set  $V_0$  is called *the crystal cell*. If the number of points in  $V_0$  is minimal among all crystal cells admissible in  $V$ , then such a cell is called the *elementary* one.

Since only the topological structure of the set is important if the percolation of random field is studied then, for the formulation of percolation theory problem, it is convenient to use the concept of *the periodic graph* and its immersion  $\mathbf{M}$  into  $\mathbb{R}^2$  defining the connectedness on the crystal lattice.

**D e f i n i t i o n 1** [4]. Let  $\Lambda = \langle V, \Phi \rangle$  be the infinite nondirectional loop-free graph where  $V$  is the set of vertexes and  $\Phi$  is the set of some two-element subsets  $\{\mathbf{x}, \mathbf{y}\} \subset V$  (edges of the graph). This graph is called the periodic one with the dimensionality 2 if it admits such an immersion  $\mathbf{M}$  into  $\mathbb{R}^2$  when the image  $\mathbf{M}V$  is the crystal lattice in  $\mathbb{R}^2$  and the image  $\mathbf{M}\Phi$  of the set  $\Phi$  is invariant relative to translations with the parallelogram of periods  $\langle \mathbf{e}_1, \mathbf{e}_2 \rangle$ ,

$$\mathbf{M}\Phi + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2 = \mathbf{M}\Phi \quad (1)$$

$\langle n_1, n_2 \rangle \in \mathbb{Z}^2$  such that the set  $\Phi_0 = \{\{\mathbf{x}, \mathbf{y}\} \in \Phi : \mathbf{M}\mathbf{y} \in V_0, \mathbf{x} \in V\}$  is finite.

If  $\{\mathbf{x}, \mathbf{y}\} \in \Phi, \mathbf{x}, \mathbf{y} \in V$ , then such vertexes are called the adjacent ones and we designate the adjacency relation between them by means of  $\mathbf{x}\phi\mathbf{y}$ .

Further, we does not distinguish vertexes of the graph and their images obtained by the immersion  $\mathbf{M}$ . We does not distinguish also immersions in  $\mathbb{R}^2$  of the graph  $\Lambda$  differing from each other. Thus, we consider that the vertex set  $V$  of the graph coincides with  $\bigcup_{\mathbf{x} \in V_0} \{\mathbb{Z}^2 + \mathbf{x}\}$  and the property (1) of its

periodicity is written down in the form  $\Phi = \Phi + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2$ . The *adjacency* relation of the periodic graph  $\langle V, \Phi \rangle$  is completely defined by the set  $\Phi_0$  since the  $\Phi$  admits the disjunctive decomposition  $\Phi = \bigcup_{\langle n_1, n_2 \rangle \in \mathbb{Z}^2} \{\Phi_0 + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2\}$ .

In this connection, we name the set  $\Phi_0$  the adjacency one. In terms of crystal physics, it defines some "nearest neighbors" on the crystal lattice of vertexes being contained in the fixed elementary crystal cell  $V_0$ .

The infinite periodic two-dimensional graph  $\Lambda$  is called the *hexagonal lattice* if its elementary cell  $V_0$  contains two vertexes. Besides, at the choice of the period parallelogram  $\langle 2\mathbf{e}_1, \mathbf{e}_1 + 3\mathbf{e}_2/2 \rangle$  defined by basis vectors  $\mathbf{e}_1, \mathbf{e}_2$  in  $\mathbb{R}^2$ , it is possible to put  $V_0 = \{\mathbf{x}_1 = \mathbf{e}_1 + \mathbf{e}_2/2, \mathbf{x}_2 = 2\mathbf{e}_1 + \mathbf{e}_2\}$  and  $\Phi_0 = \{\langle \mathbf{x}_1, \mathbf{x}_1 - \mathbf{e}_2 \rangle; \langle \mathbf{x}_1, \mathbf{x}_1 + \mathbf{e}_2/2 - \mathbf{e}_1 \rangle; \langle \mathbf{x}_1, \mathbf{x}_2 \rangle; \langle \mathbf{x}_2, \mathbf{x}_2 + \mathbf{e}_2 \rangle; \langle \mathbf{x}_2, \mathbf{x}_2 + \mathbf{e}_1 - \mathbf{e}_2/2 \rangle\}$ . The hexagonal lattice  $\langle V, \Phi \rangle$  is shown on the left-hand side of Fig.1 where the periodic structure have been represented by the dotted line on the right-hand side of it. It is formed by shifts of basis vectors of the plane using the decomposition on elementary cells which are parallelograms imposed on the lattice.

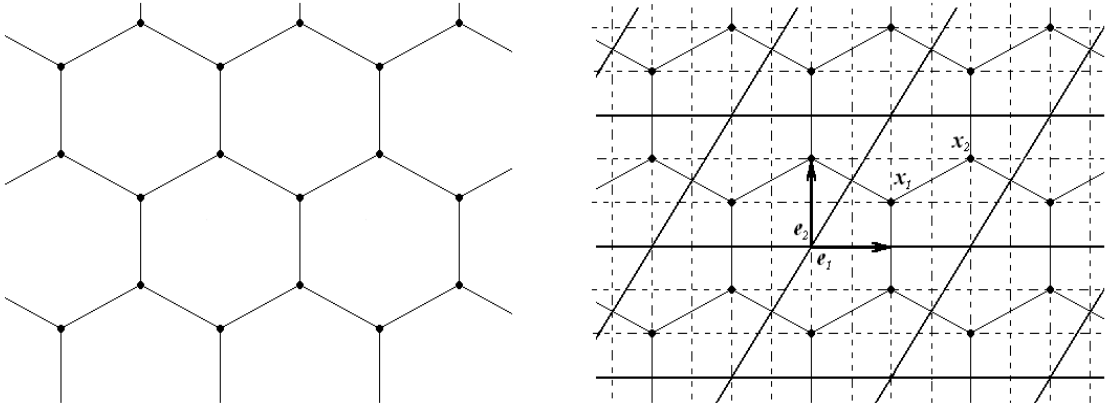


Figure 1: The hexagonal lattice.

Let us introduced into consideration the Bernoulli random field  $\{\tilde{c}(\mathbf{x}); \mathbf{x} \in V\}$  with the concentration  $c = \Pr\{\tilde{c}(\mathbf{x}) = 1\}$  on the graph  $\langle V, \Phi \rangle$ . Hereinafter, the tilde which is put over any mathematical object designates that it is random. Each random realization  $\tilde{c}(\mathbf{x}), \mathbf{x} \in V$  of the field defines the set  $\tilde{W} = \{\mathbf{x} : \tilde{c}(\mathbf{x}) = 1\}$  that we name the *configuration*. Then, the total set  $\{\tilde{c}(\mathbf{x}); \mathbf{x} \in V\}$  of random realizations together with the probability distribution

on them defines the random set on  $V$ . Its probability distribution is induced by the probability distribution of the field  $\{\tilde{c}(\mathbf{x}); \mathbf{x} \in V\}$ . Namely, for each finite subset  $M \subset V$  of lattice vertexes, the probability of their filling in the random configuration  $\tilde{W}$  is defined by the formula  $\Pr\{M \subset \tilde{W}\} = c^{|M|}$ .

The adjacency relation  $\phi$  induces the connectedness for each random configuration  $\tilde{W}$  using the concept of the way on the graph  $\langle V, \Phi \rangle$ . The sequence of vertexes  $\langle \tilde{\mathbf{x}}_0, \tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n \rangle$  chosen from the configuration  $\tilde{W}$  is called the connected way  $\alpha$  with the length  $n$  if  $\tilde{\mathbf{x}}_i \phi \tilde{\mathbf{x}}_{i+1}$ ,  $i = 0, 1, \dots, n-1$ . The way is called the simple one if  $\tilde{\mathbf{x}}_i \neq \tilde{\mathbf{x}}_j$  in the sequence pointed out at all values  $i \neq j$ ,  $i, j = 1, \dots, n$  of indexes and, accordingly, it is called the cycle if the coincidence of vertexes in the sequence  $\langle \tilde{\mathbf{x}}_0, \tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n \rangle$  takes place only at  $i = 0$ ,  $j = n$ . We name the vertex pair  $\{\mathbf{x}, \mathbf{y}\}$  the *connected* one on  $\tilde{W}$  if  $\{\mathbf{x}, \mathbf{y}\} \subset \tilde{W}$  and there is a simple way  $\alpha = \langle \mathbf{x}, \tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_{n-1}, \mathbf{y} \rangle$  on this configuration. The connectedness of all vertex pairs is the equivalence relation. Therefore, any random configuration  $\tilde{W}$  is broken up the family  $\mathfrak{M}[\tilde{W}] = \{\tilde{W}_j; j \in \mathbb{N}\}$  of not intersected and connected

sets,  $\tilde{W} = \bigcup_{j=1}^{\infty} \tilde{W}_j$ , which are called *clusters*. Each cluster consists of vertexes

connected among themselves and any two vertexes being taken from different clusters are not connected. We designate the cluster of the family  $\mathfrak{M}[\tilde{W}]$  which contains the vertex  $\mathbf{x} \in V$  by means of  $\tilde{W}(\mathbf{x})$ . If the vertex  $\mathbf{x}$  is not contained in the configuration  $\tilde{W}$  we consider that  $\tilde{W}(\mathbf{x}) = \emptyset$ .

The following random function  $\tilde{a}(\mathbf{x})$  describes the percolation property of the random field  $\{\tilde{c}(\mathbf{z}), \mathbf{z} \in V\}$ ,

$$\tilde{a}(\mathbf{x}) = \begin{cases} 1; & \text{if } |\tilde{W}(\mathbf{x})| = \infty, \\ 0; & \text{if } |\tilde{W}(\mathbf{x})| < \infty \end{cases}$$

where the designation  $|\cdot| \equiv \text{Card}(\cdot)$  is hereinafter used. In the first case, there is an infinite simple way  $\alpha(\mathbf{x}) = \langle \mathbf{x}_i; i \in \mathbb{N}_+ \rangle$  where  $\mathbf{x} = \mathbf{x}_0$  and  $\mathbf{x}_i \in \tilde{W}(\mathbf{x})$ ,  $i \in \mathbb{N}_+$ . In the second case, such a way is absent. On the basis of the random function  $\tilde{a}(\mathbf{x})$ , we may define the probability of the percolation from the fixed vertex  $\mathbf{y} \in V$  for the field  $\{\tilde{c}(\mathbf{z}); \mathbf{z} \in V\}$ . They say that the percolation from this vertex takes place if the probability  $Q(c) = \Pr\{\tilde{a}(\mathbf{y}) = 1\}$  is positive. This probability does not depend on the vertex  $\mathbf{y}$  if the periodic graph is uniform (for each pair  $\mathbf{x}, \mathbf{y} \in V$ , there are such two immersions  $\mathbf{M}_1, \mathbf{M}_2$  in  $\mathbb{R}^2$  that their images coincide with each other and  $\mathbf{M}_1\mathbf{x} = \mathbf{M}_2\mathbf{y}$ ). In the present work, we are interesting of the value  $c_* = \inf\{c : Q(c) > 0\}$  which is called the *percolation*

threshold.

**3. Finite clusters on the hexagonal lattice.** Following [4], we introduce the concept of the *external border* of the finite cluster  $\tilde{W}(\mathbf{x})$ . For this aim, we build another periodic graph  $\Lambda^* = \langle V, \Phi^* \rangle$  on the set  $V$  which is called the conjugate one to the graph  $\Lambda$ . The adjacency relation  $\Phi^*$  on the graph  $\Lambda^*$  is introduced as it is shown on Fig.2 where all vertexes being  $\phi^*$ -adjacent with the fixed vertex  $\mathbf{0}$  are pointed out. They are numbered clockwise. This mean that vertexes

$$\{\mathbf{x}_2 + \mathbf{e}_2, \mathbf{x}_2 + \mathbf{e}_1 + 3\mathbf{e}_2/2, \mathbf{x}_2 + \mathbf{e}_2 + 2\mathbf{e}_1, \mathbf{x}_2 + 2\mathbf{e}_1, \mathbf{x}_2 + \mathbf{e}_1 - \mathbf{e}_2/2, \mathbf{x}_2 + \mathbf{e}_1 - 3\mathbf{e}_2/2,$$

$\mathbf{x}_2 - 2\mathbf{e}_2, \mathbf{x}_2 - \mathbf{e}_1 - 3\mathbf{e}_2/2, \mathbf{x}_2 - \mathbf{e}_1 - \mathbf{e}_2/2, \mathbf{x}_2 - 2\mathbf{e}_1, \mathbf{x}_2 - 2\mathbf{e}_1 + \mathbf{e}_2, \mathbf{x}_2 - \mathbf{e}_1 + 3\mathbf{e}_2/2\}$  are  $\phi^*$ -adjacent with the vertex  $\mathbf{x}_2$  on Fig.1 at the used immersion of the hexagonal lattice.

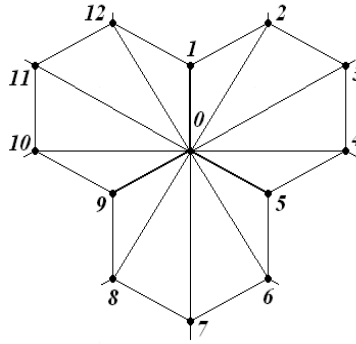


Figure 2: The adjacency relation of the vertex  $\mathbf{0}$ .

The adjacency relation  $\phi^*$  as well as the relation  $\phi$  generates the connectedness for each random configuration  $\tilde{W}$ . It breaks up both the configuration  $\tilde{W}$  and the configuration  $V \setminus \tilde{W}$  being additional to it into some connected sets.

**D e f i n i t i o n 2** [4]. *Let  $W$  be the finite cluster. The set  $\partial W$  is called the external border of  $W$  on the configuration  $\tilde{W}$  if  $W \subset \tilde{W}$  and  $\partial W$  consists of all vertexes  $\mathbf{z} \in \mathbb{Z}^2 \setminus \tilde{W}$  having the following properties.*

1. *For each  $\mathbf{z}$ , there is the vertex  $\mathbf{y} \in W$  such that  $\mathbf{z}\phi\mathbf{y}$ .*
2. *For the pointed out vertex  $\mathbf{z}$ , there exists the infinite  $\phi$ -way  $\alpha$  on the graph  $\langle V, \Phi \rangle$ ,  $\alpha \cap W = \emptyset$  which is begun from this vertex and it is unique in the intersection  $\alpha \cap \{\mathbf{x} \notin W : \mathbf{x}\phi\mathbf{y}, \mathbf{y} \in W\}$ .*

The following statement is valid.

**Theorem 1.** *Let  $W(\mathbf{x})$  be the finite cluster containing the vertex  $\mathbf{x} \in V$ . Then  $W(\mathbf{x})$  has the nonempty finite external border  $\partial W(\mathbf{x})$  which possesses the following properties.*

1. *The set  $\partial W(\mathbf{x})$  is the simple cycle on the graph  $\langle V, \Phi^* \rangle$ .*
2. *The cycle  $\partial W(\mathbf{x})$  surrounds the vertex  $\mathbf{x}$  at the periodic immersion  $\langle V, \Phi^* \rangle$  into  $\mathbb{R}^2$ .*

Although this statement is obvious, nevertheless, its full proof uses the so-called Jordan topological theorem [4].

The way simplicity property is inconvenient to express analytically. Therefore, the estimate proposed below in the item 6 is based on the revealing of suitable sufficient conditions which are guaranteed that the fixed way forms the cluster external border. Using these conditions, we will find the number estimate of external borders of all possible finite clusters containing the given vertex.

**4. The cluster decomposition on  $\mathbb{Z}^2$ .** Let  $\mathbf{A}$  be the family of finite clusters  $W$  containing the vertex  $\mathbf{0}$  of the hexagonal lattice. For each such a nonempty cluster  $W$ , we define the random event  $A(W) = \{\tilde{W} : \mathbf{0} \in \tilde{W}, W \in \mathfrak{M}[\tilde{W}], \tilde{W}(\mathbf{0}) = W\}$ . The probability of this event is equal to

$$\Pr\{A(W)\} = c^{|W|}(1 - c)^{|\partial W|}. \quad (2)$$

According to Theorem 1, for each cluster  $W$  of the family  $\mathbf{A}$ , there is the simple  $\phi^*$ -cycle belonging to the family  $\mathbf{B} = \{\gamma = \partial W; W \in \mathbf{A}\}$ . For each  $\phi^*$ -cycle  $\gamma \in \mathbf{B}$ , we define the event  $B(\gamma) = \{\tilde{M} : \mathbf{0} \in \tilde{M}, \tilde{W}(\mathbf{0}) \in \mathfrak{M}[\tilde{W}], \partial \tilde{W}(\mathbf{0}) = \gamma\}$  which is represented in the form of the following finite union of disjoint events

$$B(\gamma) = \bigcup_{W \in \mathbf{A} : \partial W = \gamma} A(W). \quad (3)$$

The probability  $P(\gamma) = \Pr\{B(\gamma)\}$  is equal to

$$P(\gamma) = \sum_{W \in \mathbf{A} : \partial W = \gamma} \Pr\{A(W)\} = \sum_{W \in \mathbf{A} : \partial W = \gamma} c^{|W|}(1 - c)^{|\partial W|}$$

according to (2) and (3).

It is valid the disjoint decomposition  $\{\tilde{a}(\mathbf{0}) = 0\} = \bigcup_{W \in \mathbf{A}} A(W)$ . The family  $\mathbf{A}$  is decomposed on some nonintersecting classes consisting of clusters joined

by the following property. We refer clusters  $W \in \mathbf{A}$  to the same class if they have the coinciding external border. Therefore, it is valid the transformation

$$\bigcup_{W \in \mathbf{A}} \dots = \bigcup_{\gamma \in \mathbf{B}} \left( \bigcup_{W \in \mathbf{A} : \partial W = \gamma} \dots \right).$$

Further, on the basis of (3), it follows that  $\{\tilde{a}(\mathbf{0}) = 0\} = \left( \bigcup_{\gamma \in \mathbf{B}} B(\gamma) \right) \cup \{\mathbf{0} \notin \tilde{W}\}$ . Thus, noticing that  $\Pr\{\mathbf{0} \notin \tilde{W}\} = 1 - c$  and  $\Pr\{\tilde{a}(\mathbf{0}) = 0\} = 1 - Q(c)$ , we come to the following statement.

**T h e o r e m 2.** *The probability  $1 - Q(c)$  is represented by the cluster decomposition*

$$1 - Q(c) = \sum_{\gamma \in \mathbf{B}} P(\gamma) + 1 - c. \quad (4)$$

The cluster decomposition (4) is converged according to its definition. But the function  $Q(c)$  is differed from zero only at  $c > c_* > 0$  and, therefore, it is not analytic. Some principle difficulties of the value  $c_*$  calculation are connected with this surcumstance. At present time, there are not some algorithms of its evaluation not using the stochastic modeling.

**5. The estimate of percolation probability.** For reception of the upper estimate of the percolation threshold, it is necessary to obtain the suitable estimate of the probability  $Q(c)$  from below. Such an estimate is based on the following statement

**L e m m a 1.** *It is valid the inequality*

$$c - Q(c) \leq \sum_{n=3}^{\infty} (1 - c)^n r_n \quad (5)$$

where  $r_n = |\{\gamma \in \mathbf{B} : |\gamma| = n\}|$ ,  $n \geq 3$ .

□ We use the elementary upper estimate  $P(\gamma) \leq (1 - c)^{|\gamma|}$  which follows from Definition 2 and the expression of  $B(\gamma)$ . Using this estimate and (4), we come to the upper restriction of the sum

$$\sum_{\gamma \in \mathbf{B}} P(\gamma) \leq \sum_{\gamma \in \mathbf{B}} (1 - c)^{|\gamma|} = \sum_{k=3}^{\infty} (1 - c)^k r_k. \quad \blacksquare$$

Now, we find the upper estimate of the value  $r_n$ ,  $n \geq 3$ . With this aim, we introduce the class  $\mathbf{B}_n$  of all such simple  $\phi^*$ -cycles with the length  $n$  on the lattice  $\Lambda^*$  that each of them surrounds the point  $\mathbf{0}$ . Further, we introduce the set  $\mathbf{C}_n(\mathbf{x}_0)$  of simple ways  $\gamma = \langle \mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_n \rangle$  on the lattice  $\Lambda^*$  having the length  $n$  and such that each of them possesses the property  $\mathbf{x}_j \neq \mathbf{x}_{j+2}$ ,  $j = 0, 1, \dots, n-2$ . We consider also those subsets  $\mathbf{C}_{n-1}(\mathbf{x}_0, \mathbf{x}_1)$  of the last introduced set  $\mathbf{C}_n(\mathbf{x}_0)$  which consist of ways having two leading fixed vertexes  $\mathbf{x}_0, \mathbf{x}_1$ . Besides, each way of these subsets is such that each two its edges following one after another, are necessarily a part of the cycle belonging to the family  $\mathbf{B} = \bigcup_{n=3}^{\infty} \mathbf{B}_n$ . In view of the uniformity of the hexagonal lattice (i.e. the equivalence of all its vertexes), the value  $|\mathbf{C}_{n-1}(\mathbf{x}_0, \mathbf{x}_1)|$  does not depend on the vertex  $\mathbf{x}_0$ .

Let  $\alpha_k = \langle \mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_k \rangle$  is the fixed simple way such that it is the part of circle belonging to the class  $\mathbf{B}$ . Further,  $\mathbf{D}(\alpha_k)$  is the set of edges  $\langle \mathbf{x}_k, \mathbf{x}_{k+1} \rangle$  such that ways  $\alpha_{k+1} = \langle \mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_k, \mathbf{x}_{k+1} \rangle$  possess the same property as the way  $\alpha_k$  has. Denote  $n_* = \max_{\alpha_k} \{|\mathbf{D}(\alpha_k)|\}$ .

*L e m m a 2. It is valid the inequality*

$$r_n < n_*(n-2) \max_{\mathbf{x}_1: \mathbf{x}_1 \phi^* \mathbf{x}_0} \{|\mathbf{C}_{n-1}(\mathbf{x}_0, \mathbf{x}_1)|\}. \quad (6)$$

□ Let us consider an infinite simple way  $\alpha(\mathbf{0})$  from the vertex  $\mathbf{0}$  on the lattice  $\Lambda$ . For definiteness, this way is chosen in such a manner that each its finite part has the least length among all ways connecting its ends. According to Theorem 1, each cycle  $\gamma$  on  $\Lambda^*$  has necessarily the vertex which is common with  $\alpha(\mathbf{0})$ . Among all such vertexes, we choose the vertex being the nearest one to the vertex  $\mathbf{0}$  where the distance is counted along the way  $\alpha(\mathbf{0})$ . We designate this vertex by  $\mathbf{z}_\gamma$ . Then, each cycle  $\gamma \in \mathbf{B}$  is contained in the unique class among not intersected classes  $\mathbf{B}(l)$ ,  $l \in \mathbb{N}$ . Each class  $\mathbf{B}(l)$  of the last family contains only those cycles  $\gamma$  of  $\mathbf{B}$  which have the correspondent vertex  $\mathbf{z}_\gamma$  at the distance  $l$  along the way  $\alpha(\mathbf{0})$ ,  $\text{dist}(\mathbf{z}_\gamma, \mathbf{0}) = l$ . On the basis of classes  $\mathbf{B}(l)$ ,  $l \in \mathbb{N}$ , we construct some classes  $\mathbf{B}_n(l) = \mathbf{B}(l) \cap \mathbf{B}_n = \{\gamma \in \mathbf{B} : |\gamma| = n, \text{dist}(\mathbf{z}_\gamma, \mathbf{0}) = l\}$ ,  $n = 3, 4, \dots, l \in \mathbb{N}$ . It is obvious that the inequality  $l \leq n-2$  takes place and,



therefore, it is valid  $\mathbf{B}_n = \bigcup_{l=1}^{n-2} \mathbf{B}_n(l)$ ,

$$r_n = \sum_{l=1}^{n-2} |\mathbf{B}_n(l)|. \quad (7)$$

Let us fix the clockwise direction on cycles  $\gamma = \langle \mathbf{z}_\gamma, \mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{z}_\gamma \rangle$  of  $\mathbf{B}_n(l)$ . We introduce into consideration disjointed sets  $\mathbf{B}_n(l, \mathbf{a}) = \{\gamma \in \mathbf{B}_n(l) : \mathbf{x}_1 - \mathbf{z}_\gamma = \mathbf{a}\}$  of cycles containing in  $\mathbf{B}_n(l)$  such that each of them has the fixed leading vertex that follows after  $\mathbf{z}_\gamma$  according to the direction on  $\gamma$ . This vertex is  $\mathbf{x}_1 = \mathbf{z}_\gamma + \mathbf{a}$ . The vector  $\mathbf{a}$  is one of vectors on Fig.2 provided that  $\mathbf{z}_\gamma$  is translated to  $\mathbf{0}$ . Then, the disjoint decomposition  $\mathbf{B}_n(l) = \bigcup_{\mathbf{y}: \mathbf{z}_\gamma \phi^* \mathbf{y}} \mathbf{B}_n(l, \mathbf{y} - \mathbf{z}_\gamma)$

takes place and, therefore,

$$|\mathbf{B}_n(l)| = \sum_{\mathbf{y}: \mathbf{z}_\gamma \phi^* \mathbf{y}} |\mathbf{B}_n(l, \mathbf{y} - \mathbf{z}_\gamma)|. \quad (8)$$

It is obvious that  $|\mathbf{B}_n(l, \mathbf{a})| \leq |\mathbf{C}_{n-1}(\mathbf{z}_\gamma, \mathbf{z}_\gamma + \mathbf{a})|$ . Namely, any fixed circle of  $\mathbf{B}_n(l, \mathbf{a})$  turns to the way of  $\mathbf{C}_{n-1}(\mathbf{z}_\gamma, \mathbf{z}_\gamma + \mathbf{a})$  after the removal of the last circle edge according to the order. Thus, we obtain the injection since no more than one cycle of  $\mathbf{B}_n(l, \mathbf{a})$  corresponds to each way of  $\mathbf{C}_{n-1}(\mathbf{z}_\gamma, \mathbf{z}_\gamma + \mathbf{a})$ . Thus, on the basis of the above estimate and (8), it follows the inequality

$$|\mathbf{B}_n(l)| \leq n_* \max_{\mathbf{x}_1: \mathbf{x}_1 \phi^* \mathbf{x}_0} \{|\mathbf{C}_{n-1}(\mathbf{x}_0, \mathbf{x}_1)|\}.$$

Since the value  $|\mathbf{C}_{n-1}(\mathbf{x}_0, \mathbf{x}_1)|$  does not depend on  $l = \text{dist}(\mathbf{0}, \mathbf{z}_\gamma)$ , we obtain (6) applying the received inequality to do the upper estimate of the right-hand side of the decomposition (7). ■

We introduce the construction for the estimating of the value  $|\mathbf{C}_{n-1}(\mathbf{x}_0, \mathbf{x}_1)|$ . We characterize uniquely each way of  $\mathbf{C}_n(\mathbf{x}_0)$ ,  $n \geq 2$  by the sequence  $\langle \mathbf{a}_1, \dots, \mathbf{a}_{n-1} \rangle$  of *shift* vectors where  $\mathbf{a}_1 = \mathbf{x}_1 - \mathbf{x}_0$  and each its vector  $\mathbf{a}_i$ ,  $i = 2, \dots, n$  represents the vector  $\mathbf{x}_i - \mathbf{x}_{i-1}$  turned on the angle being least among two ones formed by the vector  $\mathbf{x}_{i-1} - \mathbf{x}_{i-2}$  and the basis vector  $\mathbf{e}_2$  on the lattice plane. Now, we introduce the set  $\mathbf{G}_n(\mathbf{a}_1)$  of all sequences  $\langle \mathbf{a}_1, \dots, \mathbf{a}_n \rangle$  with the fixed vector  $\mathbf{a}_1$  and such that each pair  $\langle \mathbf{a}_i, \mathbf{a}_{i+1} \rangle$ ,  $i = 1, 2, \dots, n-1$  is admissible in it. Here, the pair  $\langle \mathbf{a}, \mathbf{a}' \rangle$  is called the admissible one if there exists the circle  $\gamma$  in the family  $\mathbf{B}$  such that the corresponding sequence contains the pair  $\langle \mathbf{a}, \mathbf{a}' \rangle$  of vectors

following one after another in it. The introduced set is equivalent to the set  $\mathbf{C}_n(\mathbf{x}_0, \mathbf{x}_1)$ . Hence,  $|\mathbf{C}_n(\mathbf{x}_0, \mathbf{x}_1)| = g(\mathbf{a}_1; n) \equiv |\mathbf{G}_n(\mathbf{a}_1)|$ .

Let us decompose the set  $\mathbf{G}_n(\mathbf{a}_1)$  by the following way  $\mathbf{G}_n(\mathbf{a}_1) = \bigcup_{\mathbf{a}_n} \mathbf{G}_n(\mathbf{a}_1; \mathbf{a}_n)$  on not intersecting sets  $\mathbf{G}_n(\mathbf{a}_1; \mathbf{a}_n)$  of sequences  $\langle \mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n \rangle$  where the last shift vector  $\mathbf{a}_n$  is fixed side by side the first one. Then,  $g(\mathbf{a}_1; n) = \sum_{\mathbf{a}_n} |\mathbf{G}_n(\mathbf{a}_1, \mathbf{a}_n)|$ .

Introducing the numbering for possible shift vectors which is presented on Fig.2, we may consider that the value  $\langle |\mathbf{G}_n(\mathbf{a}_1, \mathbf{a}_n)| = g_j(\mathbf{a}_1, n); j = 1 \div 12 \rangle$  is 12-dimensional vector for each  $n \in \mathbb{N}$ . Here, the component number  $j = 1 \div 12$  is defined by the number of the shift vector  $\mathbf{a}_n$  in the accepted numbering.

Thus,  $g(\mathbf{a}_1; n) = \sum_{j=1}^{12} g_j(\mathbf{a}_1; n)$ .

Now, let us define the matrix  $\mathcal{S}$  with the dimension equal to the number of nearest neighbors of the vertex on the conjugate lattice  $\Lambda^*$ . For the hexagonal lattice, this number is equal to 12. Matrix elements  $S_{ij}$ ,  $i, j = 1 \div 12$  may have values 0 or 1 according to the following rule. We put  $S_{ij} = 1$  if there is such a pair  $\langle \mathbf{a}_k, \mathbf{a}_{k+1} \rangle$  of shift vectors at  $k = 1, \dots, n-1$  in one of a sequence in the set  $\mathbf{G}_n(\mathbf{a}_1, \mathbf{a}_n)$  for anything value  $n = 3, 4, \dots$  and vectors  $\mathbf{a}_k, \mathbf{a}_{k+1}$  have numbers  $i$  and  $j$  according to the numbering accepted on Fig.2. On the contrary,  $S_{ij} = 0$  if there is not the circle with the external border which contains the pointed out joining of edges. Further, we will name the matrix  $\mathcal{S}$  as *the matrix of way connection*. Since  $S_{ij} \geq 0$ ;  $i, j = 1 \div 12$ , then its maximal modulo eigenvalue  $\lambda_0$  is positive according to the Frobenius theorem (see, [7]) for matrixes with nonnegative elements.

**L e m m a 3.** *Let the matrix  $\mathcal{S}$  has the unique eigenvalue  $\lambda_0 > 0$  with maximal modulus. Then, the asymptotic formula*

$$g_i(\mathbf{a}_1, n) = C_{ij} \lambda_0^{n-1} (1 + o(1)), \quad n \rightarrow \infty \quad (9)$$

*takes place where the number  $j$  corresponds to the shift vector  $\mathbf{a}_1$  and the nonzero matrix  $\mathcal{C}$  has non-negative matrix elements  $C_{ij}$ .*

□ According to the definition of the vector  $\langle g_i(\mathbf{a}_1; n); j = 1 \div 12 \rangle$ , the recurrent relation

$$g_i(\mathbf{a}_1; n) = \sum_{k=1}^{12} g_k(\mathbf{a}_1; n-1) S_{ki}$$

takes place for any  $n = 2, 3, \dots$  and for the vector  $\mathbf{a}_1$  with number  $j$ . Besides, it

takes place  $g_i(\mathbf{a}_1; 1) = S_{ji}$ . Then, using the induction on  $n \in \mathbb{N}$ , we conclude that

$$g_i(\mathbf{a}_1; n) = (\mathcal{S}^{n-1})_{ji}.$$

Since the matrix  $\mathcal{S}$  has the unique eigenvalue  $\lambda_0$  with the maximal absolute value, for the expression in the right-hand side of last equality, the asymptotic formula (9) is valid at  $n \rightarrow \infty$ . Besides,  $S_{ij} \geq 0$  and, hence, the nonnegativity of matrix elements  $C_{ij}$  follows from the Frobenius theorem. ■

Now, we may find the below estimate of the probability  $Q(c)$ .

**T h e o r e m 3.** *Let the maximal eigenvalue  $\lambda_0$  of the matrix  $\mathcal{S}$  of way connections be unique. Then, it is valid the following below estimate of the probability  $Q(c)$*

$$Q(c) \geq c - n_*(1-c)^2 \sum_{l=3}^{\infty} (n-2)[(1-c)\lambda_0]^{n-2}. \quad (10)$$

□ On the basis of Lemmas 1 and 2 and the definition of the functions  $g_i(\mathbf{a}_1; n)$ ,  $i = 1 \div 12$ , we have

$$\begin{aligned} c - Q(c) &\leq \sum_{n=3}^{\infty} (1-c)^n r_n \leq n_* \sum_{n=3}^{\infty} (n-2)(1-c)^n \max_{\mathbf{x}_1} \{|\mathbf{C}_{n-1}(\mathbf{x}_0, \mathbf{x}_1)|\} = \\ &= n_* \sum_{n=3}^{\infty} (n-2)(1-c)^n g_{n-1}(\mathbf{a}_1) = n_* \sum_{n=3}^{\infty} (n-2)(1-c)^n \sum_{i=1}^{12} g_i(\mathbf{a}_1; n-1). \end{aligned}$$

Applying the asymptotic formula (9), we obtain

$$c - Q(c) \leq n_* C (1-c)^2 \sum_{n=3}^{\infty} (n-2)[(1-c)\lambda_0]^{n-2}$$

where the positive constant  $C > \max_j \sum_{i=1}^{12} C_{ij}$  is chosen by such a way that the inequality  $g_i(\mathbf{a}_1, n) < C\lambda_0^{n-1}$ ,  $n \in \mathbb{N}$  takes place. ■

**C o r o l l a r y.** *For the percolation threshold  $c_*$  of the Bernoulli random field  $\{\tilde{c}(\mathbf{x}); \mathbf{x} \in V\}$  on the hexagonal lattice  $\langle V, \Phi \rangle$ , the inequality  $c_* \leq 1 - \lambda_0^{-1}$  is valid.*

□ The series in the right-hand side of the inequality (10) converges at  $(1-c)\lambda_0 < 1$ . Then, it takes place at  $c > 1 - \lambda_0^{-1}$ . The convergence of

this series, applying the reasoning based on the Borel-Cantelli lemma (see, for example, [8]) leads to the percolation probability  $Q(c)$  being distinct from zero. It takes place at the above pointed out restriction on the parameter  $c$ . Hence,  $c_* \leq 1 - \lambda_0^{-1}$ . ■

**6. The upper estimate of the percolation threshold.** It follows from considerations of the previous section that the problem of the upper estimation of the percolation threshold on the hexagonal lattice is reduced to calculation of the eigenvalue  $\lambda_0$ . For its calculation, first of all, it is necessary to find the matrix  $\mathcal{S}$ . For the evaluation of matrix elements  $S_{ij}$ , it is necessary either to find the cluster which has the external border containing the pair of edges  $\langle \mathbf{a}, \mathbf{a}' \rangle$  where vectors  $\mathbf{a}, \mathbf{a}'$  have numbers  $i$  and  $j$  correspondingly or to prove that there is not the cluster with such a pair. Following statements describe the general structure of the matrix  $\mathcal{S}$  and point out its zero elements.

*L e m m a 4. The matrix  $S_{ij}$  is symmetric and  $S_{ii} = 0$ .*

□ Since the passage of the cycle being the external border is possible in both directions, the existence or the absence of pair edges  $\langle \mathbf{a}, \mathbf{a}' \rangle$  following one after another in it which have numbers  $i$  and  $j$  correspondingly leads to existence or absence of the cycle which has the pair of edges  $\langle \mathbf{a}', \mathbf{a} \rangle$ . It means that  $S_{ij} = S_{ji}$ .

The equality  $S_{ii} = 1$  corresponds to the fact that there is the pair of edges in the external border which are described by the pair  $\langle \mathbf{a}, \mathbf{a} \rangle$  of shift vectors in the sequence  $\langle \mathbf{a}_1, \dots, \mathbf{a}_n \rangle$  and the vector  $\mathbf{a}$  has number  $i$ . It means, according to the description of the cycle by means of the specified sequence that these edges look as  $\langle \mathbf{x}, \mathbf{y} \rangle$  and  $\langle \mathbf{y}, \mathbf{x} \rangle$ . But it is impossible. Therefore,  $S_{ii} = 0$  for all values  $i = 1 \div 12$ . ■

*L e m m a 5. The Matrix  $S_{ij}$  has the property  $S_{1,j} = S_{1,14-j}$ ,  $S_{5,j} = S_{5,10-j}$ ,  $S_{9,j} = S_{9,18-j}$ ,  $j = 2 \div 12$  where the subtraction operation in bottom indexes is understood modulo 12.*

□ The first relation follows from the symmetry of Fig.2 describing the joining of edges in the vertex **0** relative to the reflection from the straight line defined by vertexes **1, 0, 7**. The second relation follows from the symmetry of this figure to the reflection from the straight line passing through vertexes **5, 0, 11** and the third relation is connected with the reflection from the straight line passing through vertexes **3, 0, 9**. ■

*L e m m a 6. Matrix elements  $S_{ij}$  have the property  $S_{i+4,j+4} = S_{ij}$  where*

sums  $i + 4$  and  $j + 4$  are understood modulo 12.

□ This property follows from the symmetry of Fig.2 describing all possible connections of edges in the vertex **0** relative to rotations on the angle  $2\pi/3$ . ■

*C o r o l l a r y.* The matrix  $\mathcal{S}$  has the following block structure made of two  $4 \times 4$ -matrices  $F, G$

$$\mathcal{S} = \begin{pmatrix} F & G & G^+ \\ G^+ & F & G \\ G & G^+ & F \end{pmatrix}. \quad (11)$$

□ Using  $4 \times 4$ -matrices  $F, G, H$  with matrix elements  $F_{ij} = S_{ij}$ ,  $G_{ij} = S_{i,j+4}$ ,  $H_{ij} = S_{i,j+8}$ ,  $i, j = 1 \div 4$ , it follows from Lemma 6 that the matrix  $\mathcal{S}$  is represented as

$$\mathcal{S} = \begin{pmatrix} F & G & H \\ H & F & G \\ G & H & F \end{pmatrix}.$$

From Lemma 4, it follows that  $H = G^+$ , as  $G_{ij} = S_{i,j+4} = S_{i+8,j}$  at  $i, j = 1 \div 4$  and, simultaneously,  $S_{i+8,j} = S_{j,i+8} = H^+$ . ■

*L e m m a 7.*  $S_{1,5} = 0$ .

□ Each vertex  $\mathbf{x}$  of the external border  $\partial W$  should have the vertex  $\mathbf{y}$  adjacent with it and belonging to  $W$ . Besides, there exists the vertex  $\mathbf{z}$  adjacent with  $\mathbf{x}$ , but not belonging  $W \cup \partial W$ . If we admit that  $S_{1,5} = 1$ , then vertexes **1** and **5** (see, Fig.3 where joinings of edges in the vertex **0** are shown by the dotted line) belong to  $\partial W$  and, hence, they do not belong to  $W$ . Since the vertex **0** has three vertexes **1,5,9** adjacent with it, then the vertex **9** should be simultaneously the vertex of  $W$  and it does not belong to  $W \cup \partial W$ . But, it is impossible. ■

*L e m m a 8.*  $S_{ij} = 0$ ,  $i, j = 1 \div 4$ .

□ It is sufficient to prove that  $S_{1,j} = 0$ ,  $j = 2, 3, 4$  and  $S_{2,j} = 0$ ,  $j = 3, 4$ . We consider the first group of matrix elements. Vertexes **0** and **1** belong to  $\partial W$ . There are vertexes  $\mathbf{x}, \mathbf{y} \in W$  such that  $\mathbf{x} \neq \mathbf{1}$ ,  $\mathbf{y} \neq \mathbf{0}$  and also there are vertexes  $\mathbf{x}', \mathbf{y}' \notin W \cup \partial W$  such that  $\mathbf{x}' \neq \mathbf{1}$ ,  $\mathbf{y}' \neq \mathbf{0}$ . Further, there are ways from vertexes  $\mathbf{x}'$  and  $\mathbf{y}'$  to infinity not crossing  $W$ . Vertexes **2** and **12** may play the role of vertexes  $\mathbf{x}, \mathbf{x}'$  for the vertex **1** and only vertexes **5** and **9** may be the same for the vertex **0**. Then, there are four choice variants of vertex pairs  $\mathbf{x}, \mathbf{x}'$  and  $\mathbf{y}, \mathbf{y}'$  among presented possibilities. It is sufficient to analyze only two cases which

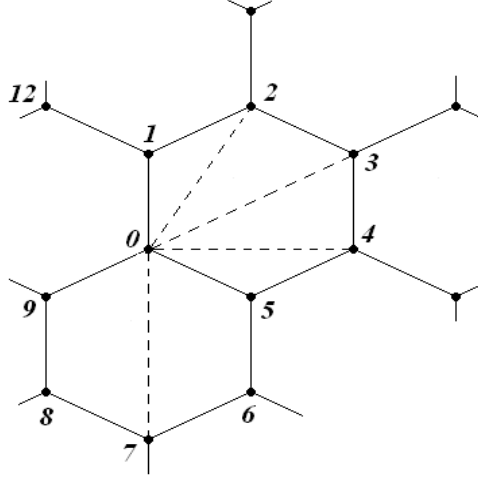


Figure 3: Possible joinings of edges in the vertex  $0$ .

do not reduce to each other by mirror reflection relative to the straight line passing through vertexes  $1, 0, 7$ . We choose the following possibilities. Vertexes  $2$  and  $12$  are the vertexes  $x, x'$  in both cases. And the vertexes  $9$  and  $5$  are the vertexes  $y, y'$  in the first case and, on the contrary, they are interchanged their position in the second.

In the first case, there are not infinite ways from vertexes  $1$  and  $0$  which are crossed with  $W$  and passed through vertexes  $12$  and  $5$  correspondingly. We consider the line in the plane where the lattice is placed. This line consists of the first infinite way of lattice edges that comes from infinity to the vertex  $12$ . Further, it consists of the sequence of edges  $\langle 12, 1 \rangle, \langle 1, 0 \rangle, \langle 0, 5 \rangle$  and it is ended by the second infinite way from the vertex  $5$  to infinity. The constructed line divides the plane into two parts so that vertexes  $x$  and  $y$  are in different ones. Then, vertexes  $x$  and  $y$  should not belong to the same cluster  $W$  since any way from the vertex  $x$  to the vertex  $y$  on lattice edges crosses necessarily this line. Besides, it may be done only in the lattice vertex. Hence, the edge connection  $\langle 1, 0 \rangle$  with one of edges  $\langle 0, j \rangle, j = 2, 3, 4$  is impossible in the variant under consideration.

In the second case, it is considered the analogous line on the plane which consists of the way coming from infinity to the vertex  $1$  without crossing of the cluster  $W$ . Further, it consists of the edge  $\langle 1, 0 \rangle$ , the diagonal of the given lattice hexagon which is led from the vertex  $0$  to the vertex  $j$  (it is presented on Fig.3 where this side has the border vertexes  $0, 1, 2, 3, 4, 5$ ) and the way

from the vertex  $\mathbf{j}$  to infinity on lattice edges without the crossing of  $W$ . The line constructed divides the plane into two parts so that vertexes  $\mathbf{x}$  and  $\mathbf{y}$  are in different ones. Therefore, they should not belong to the same cluster  $W$  since any way on lattice edges from the vertex  $\mathbf{y}$  to the vertex  $\mathbf{x}$  necessarily crosses the line in the lattice vertex.

Contradictions obtained in both cases show that  $S_{1,j} = 0$  at  $j = 2, 3, 4$ .

Let us consider the second group of matrix elements  $S_{23}, S_{24}$ . We construct the following line on the lattice plane. Firstly, it consists of the way which comes to the vertex  $\mathbf{2}$  from infinity without crossing of the cluster  $W$ . It should exist since the vertex  $\mathbf{2}$  belongs to  $\partial W$ . Further, the line consists of the consecutive passage of two diagonals on the hexagon presented on Fig.3. Diagonals are defined by vertex pairs  $\langle \mathbf{2}, \mathbf{0} \rangle$  and  $\langle \mathbf{0}, \mathbf{j} \rangle$  where  $\mathbf{j} = \mathbf{3}, \mathbf{4}$ . The line is ended by the way from the vertex  $\mathbf{j}$  to infinity. It divides the plane into two parts and the cluster  $W$  should be settled down completely in one of them.

It is obvious that  $S_{23} = 0$  since the cluster  $W$  may be not settled down on the right-hand side of the constructed line according to the direction accepted on it. Otherwise, the vertex  $\mathbf{0}$  has no vertexes belonging to  $W$  and being adjacent with it. On the other hand, the cluster  $W$  may not be on the left-hand side of this line since there is the way leaving from the vertex  $\mathbf{0}$  to infinity without crossing of the cluster  $W$ . It should exist according to the definition of the external border vertex. This way should be also in the left part of the plane. Then, the way divides the left-hand side into two parts again. The cluster  $W$  should be settled down completely in one of them and, therefore, one of vertexes  $\mathbf{2}$  or  $\mathbf{j}$  does not belong to the external border since there is not anything vertex of  $W$  adjacent to it. The obtained contradiction proves the equality  $S_{24} = 0$ . ■

*T h e o r e m 4. The matrix  $\mathcal{S}$  is presented by the formula*

$$S = \begin{pmatrix} \mathbf{0} & G & G^+ \\ G^+ & \mathbf{0} & G \\ G & G^+ & \mathbf{0} \end{pmatrix}, \quad G = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix} \quad (12)$$

where  $\mathbf{0}$  is the zero matrix.

□ It follows from Lemmas 5 and 8 that  $S_{3,4} = S_{3,2} = S_{2,3} = 0$ . Then the matrix  $F$  in the formula (11) is zero owing to Lemma 4. On the basis of the

property  $S_{1,j} = S_{1,14-j}$  and Lemmas 7 and 8, we find

$$S_{1,12} = S_{1,2} = 0; \quad S_{1,11} = S_{1,3} = 0; \quad S_{1,10} = S_{1,4} = 0; \quad S_{1,9} = S_{1,5} = 0.$$

Then, the first line in the matrix  $G^+$  in the formula (11) and, hence, the first column in the matrix  $G$  are zero. Other elements of the matrix  $G$  are equal to unity due to the above mentioned criterion at the evaluation of matrix elements. So, it is had  $S_{ij} = 1$  at  $i = 1 \div 4, j = 6, 7, 8$  (see Figs. 4-7). ■

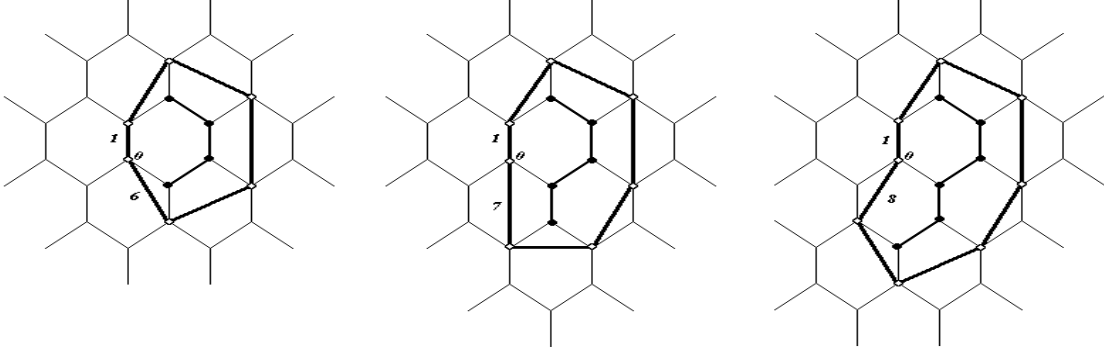


Figure 4: Clusters containing the edge **1-0**.

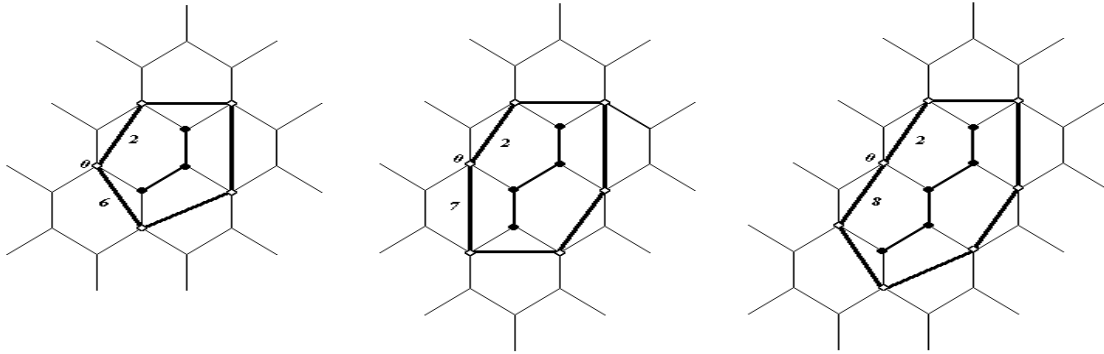


Figure 5: Clusters containing the edge **2-0**.

**N o t i c e.** It follows from the matrix  $\mathcal{S}$  expression that  $n_* = 7$ .

On the basis of Theorem II in Appendix, having put  $n = 3, m = 4, A = \mathcal{S}, A^{(1)} = \mathbf{0}, A^{(2)} = G, A^{(3)} = G^+$ , we conclude that the maximal eigenvalue  $\lambda_0$  of



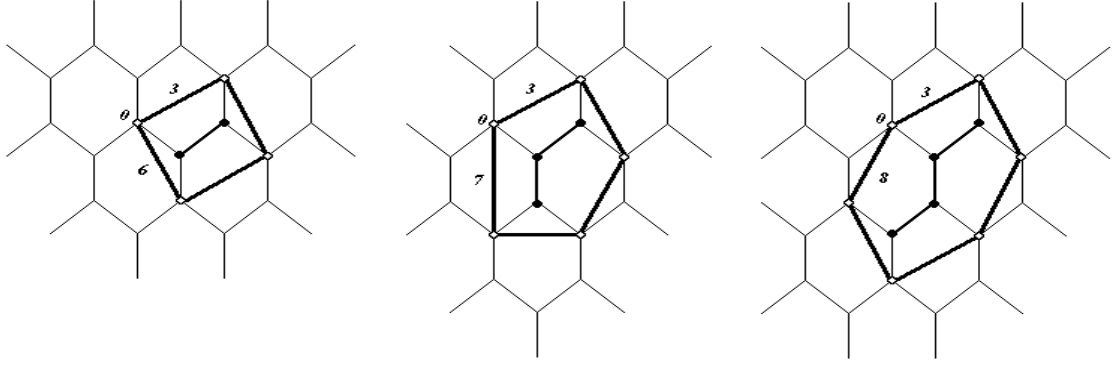


Figure 6: Clusters containing the edge **3-0**.

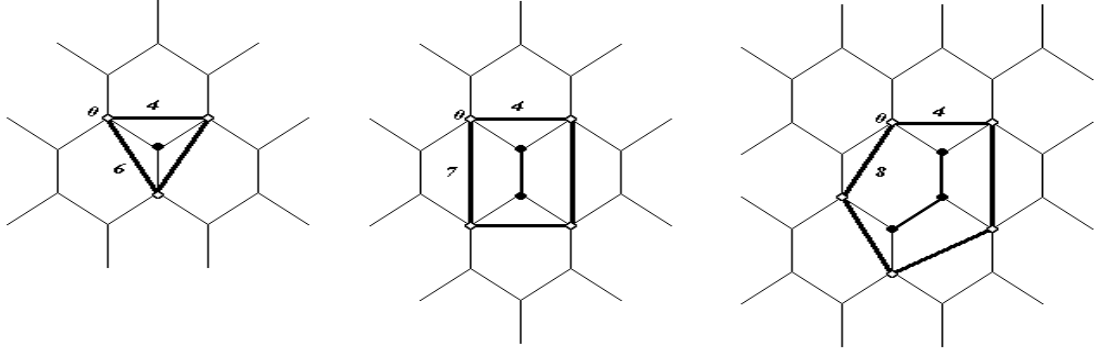


Figure 7: Clusters containing the edge **4-0**.

the matrix  $\mathcal{S}$  coincides with the maximal eigenvalue of the matrix

$$B = \mathbf{0} + G + G^+ = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 2 & 2 \end{pmatrix}$$

The rank of this matrix is obviously equal 2. Then, it has two zero eigenvalues and, therefore, its characteristic equation looks as follows

$$\det(B - \lambda \mathbf{1}) = (\lambda^2 - \lambda \xi_1 + \xi_2) \lambda^2 = 0$$

where  $\xi_1 = \text{Sp } B$ ,  $\xi_2 = [\text{Sp } B^2 - (\text{Sp } B)^2]/2$ . Then,  $\xi_1 = \text{Sp } B = 6$  and  $\xi_2 = 3$  since diagonal elements of the matrix  $B^2$  are equal  $(B^2)_{ii} = 3, 13, 13, 13$ . Hence, the number  $\lambda_0$  is the greatest root of the quadratic equation  $\lambda^2 - 6\lambda - 3 = 0$ . Whence, we obtain  $\lambda_0 = 3 + 2\sqrt{3}$ . Thus, we have proved the following statement.

**T h e o r e m 5.** *The maximal eigenvalue  $\lambda_0$  of the matrix  $\mathcal{S}$  is equal  $3 + 2\sqrt{3} \approx 6,46$ .*

From Theorem 5 and Corollary of Theorem 3, it follows directly

**The basic statement.** *The percolation threshold  $c_*$  of the Bernoulli field on the hexagonal lattice does not surpass the number  $2/3(3 - \sqrt{3})$ .*

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## Appendix

**L e m m a I.** *Let  $B$  be the  $m \times m$ -matrix with nonnegative elements such that there is the number  $\mu > 0$  and the vector  $\mathbf{b} \in \mathbb{R}^m$ ,  $\mathbf{b} = \langle b_1, \dots, b_m \rangle$  with nonnegative components such that it takes place the inequality*

$$\mu b_k \leq \sum_{l=1}^m B_{kl} b_l, \quad k = 1 \div m. \quad (A1)$$

*Then the maximal eigenvalue  $\lambda(B)$  of the matrix  $B$  on the absolute value is positive and it satisfies the inequality  $\lambda(B) \geq \mu$ .*

□ We apply  $N$  times the inequality (A1). Using the induction on  $N$ , it is obtained the inequality

$$\mu^N b_k \leq \sum_{l=1}^m (B^N)_{kl} b_l. \quad (A2)$$

At first, we prove the inequality (A1) in the case when the matrix  $B$  has only one-dimensional eigenspaces. Let  $\mathbf{c}^{(r)} = \langle c_k^{(r)}; k = 1 \div m \rangle$  be eigenvectors of the matrix  $B$  with correspondent eigenvalues  $\lambda_r$ ,  $r = 1 \div m$ . We consider that all  $\lambda_r$  have been ordered according to the decrease of their absolute values (at the coincidence of absolute values, they are ordered according to their phases). We write down the decomposition of the vector

$$\mathbf{b} = \sum_{r=1}^m \xi_r \mathbf{c}^{(r)}, \quad \xi_r \in \mathbb{C}, r = 1 \div m.$$

Then,

$$B^N \mathbf{b} = \sum_{r=1}^m \xi_r \lambda_r^N \mathbf{c}^{(r)}$$

and, therefore, the inequality (A2) is represented in the form

$$\mu^N b_k \leq \sum_{r=1}^m \xi_r \lambda_r^N c_k^{(r)}. \quad (A3)$$

There is the number  $k \leq m$  such that  $b_k > 0$ . Let us consider the inequality (A3) for this number. Among all numbers  $r = 1 \div m$ , there is the minimal number  $r_0$  such that  $\xi_{r_0} c_k^{(r_0)} \neq 0$ . Then, the inequality (A3) is rewritten in the form

$$\mu^N b_k \leq \sum_{r=r_0}^m \xi_r \lambda_r^N c_k^{(r)}$$

or, calculating the  $N$ -th degree root for both positive parts of the inequality, we obtain

$$\mu b_k^{1/N} \leq \lambda_{r_0} \left[ \sum_{r=r_0}^m \xi_r (\lambda_r / \lambda_{r_0})^N \mathbf{c}_k^{(r)} \right]^{1/N} = |\lambda_{r_0}| \left| \sum_{r=r_0}^m \xi_r (\lambda_r / \lambda_{r_0})^N \mathbf{c}_k^{(r)} \right|^{1/N}.$$

The last equality is valid due to the positivity of the right-hand side of (A3). Further, we go to the limit  $N \rightarrow \infty$ . In this case,  $\lim_{N \rightarrow \infty} b_k^{1/N} = 1$ . Due to the boundedness of the summing expression in the right-hand side of the inequality, its upper limit does not surpass the unity. Then,  $\mu \leq |\lambda_{r_0}|$ . According to the definition and due to the Frobenius theorem,  $|\lambda_{r_0}| \leq \lambda(B)$ .

One may change any matrix  $B$  by such a way that all its eigenspaces turns into one-dimensional ones. It is done by means of addition to the matrix  $B$  of the suitable matrix with nonnegative elements. It may be done as much near to zero matrix as one wants. This nearness is understood according to the  $\mathbb{R}^{m^2}$  topology. The possibility of this follows from the fact that the multiplicity condition of eigenvalues satisfying the characteristic equation  $\det(B - \lambda \mathbf{1}) = 0$  is expressed by the supplement equation  $\frac{d}{d\lambda} \det(B - \lambda \mathbf{1}) = 0$ . The last equation cuts out a differential manifold with the codimensionality one in the space  $\mathbb{R}^{m^2}$  of admissible matrices  $B$ . At such an addition of small matrix, the matrix  $B$  transforms to such a matrix  $B_\epsilon$  that  $B_\epsilon \rightarrow B$  at  $\epsilon \rightarrow +0$ .

The inequality (A1) is proved in general case by the following way. Let  $\mathbf{b}$  be the eigenvector of the matrix  $B$  corresponding to  $\lambda(B)$ . Since

$$\lambda(B) b_k = \sum_{l=1}^m B_{kl} b_l \leq \sum_{l=1}^m (B_\epsilon)_{kl} b_l$$

and the matrix  $B_\epsilon$  has only one-dimensional eigenspaces, the inequality (A1) takes place where it is needed to change both  $\lambda(B)$  on  $\lambda(B_\epsilon)$  and  $\mu$  on  $\lambda(B)$ . Consequently,  $\lambda(B) \leq \lambda(B_\epsilon)$ . After that, we come to the limit  $\epsilon \rightarrow +0$ . ■

**T h e o r e m I.** *Let  $A$  be the  $n \times n$ -matrix with nonnegative elements. It consists of  $m^2$  blocks being rectangular matrixes  $B^{(k,l)}$  which have correspondingly  $p_k$  lines and  $s_l$  columns  $k, l = 1 \div m$ ,  $m \leq n$ ,  $p_1 + p_2 + \dots + p_m = n$ ,*

$$s_1 + s_2 + \dots + s_m = n,$$

$$A = \begin{pmatrix} B^{(1,1)} & B^{(1,2)} & \dots & B^{(1,m)} \\ B^{(2,1)} & B^{(2,2)} & \dots & B^{(2,m)} \\ \vdots & \vdots & \vdots & \vdots \\ B^{(m,1)} & B^{(m,2)} & \dots & B^{(m,m)} \end{pmatrix}. \quad (A4)$$

Matrix elements of the square  $m \times m$ -matrix  $B$  are defined by the formula

$$B_{kl} = \max \left\{ \sum_{j=1}^{s_l} B_{ij}^{(k,l)}; i = 1 \div p_k \right\}, \quad k, l = 1 \div m.$$

Then, positive eigenvalues  $\lambda(A)$  and  $\lambda(B)$  corresponding to matrixes  $A$  and  $B$  which are maximal on their absolute values satisfy the inequality  $\lambda(B) \geq \lambda(A)$ .

□ Matrixes  $A$  and  $B$  possess nonnegative elements. Due to the Frobenius theorem [7], eigenvalues of these matrixes are positive if they are maximal on their absolute values. Besides, due to this theorem, there are such eigenvectors of matrixes  $A$  and  $B$  corresponding to eigenvalues pointed out that they have nonnegative components. We designate them as follows  $\mathbf{a} = \langle a_1, \dots, a_n \rangle$ ,  $a_j \geq 0$ ,  $j = 1 \div n$ ;  $\mathbf{b} = \langle b_1, \dots, b_m \rangle$ ,  $b_i \geq 0$ ,  $i = 1 \div m$ . Then,

$$\sum_{j=1}^n A_{ij} a_j = \lambda(A) a_i, \quad \sum_{l=1}^m B_{kl} b_l = \lambda(B) b_k.$$

We introduce the vector  $\mathbf{c} \in \mathbb{R}^m$ ,  $\mathbf{c} = \langle c_1, \dots, c_m \rangle$  with components  $c_k = \max\{a_i; s_1 + \dots + s_{k-1} < i \leq s_1 + \dots + s_k\}$ . Dividing summations on  $j = 1 \div n$  in both sides of first equality, we introduce repeated summations. First of them is done on groups containing  $s_1, \dots, s_m$  numbers, the second is done within each of these groups. In a result, we obtain

$$\sum_{j=1}^n A_{ij} a_j = \sum_{l=1}^m \sum_{j=s_1+\dots+s_{l-1}+1}^{s_1+\dots+s_l} A_{ij} a_j \leq \sum_{l=1}^m c_l \sum_{j=s_1+\dots+s_{l-1}+1}^{s_1+\dots+s_l} A_{ij}.$$

Using the change  $i \Rightarrow p_1 + \dots + p_{k-1} + i$ ,  $i = 1 \div p_k$ , we rewrite the last inequality in the form

$$\lambda(A) a_{i+p_1+\dots+p_{k-1}} \leq \sum_{l=1}^m c_l \sum_{j=1}^{s_l} B_{i,j}^{(k,l)}.$$

Calculating the maximum on  $i$  in both sides of the inequality, we obtain

$$\lambda(A)c_k \leq \sum_{l=1}^m B_{k,l}c_l. \quad (A5)$$

The last inequality coincides with (A1), if we put  $\mu = \lambda(A)$  and change  $\mathbf{b}$  on  $\mathbf{c}$ . Then, the theorem statement follows from (A1). ■

**T h e o r e m II.** *Let  $\langle A^{(1)}, \dots, A^{(n)} \rangle$  be the ordered collection of  $m \times m$ -matrixes with nonnegative elements. Further, let  $nm \times nm$ -matrix  $A$  be made up of  $m \times m$ -matrixes  $B^{(k,l)}$  according to the following formula*

$$A = \begin{pmatrix} B^{(1,1)} & B^{(1,2)} & \dots & B^{(1,n)} \\ B^{(2,1)} & B^{(2,2)} & \dots & B^{(2,n)} \\ \vdots & \vdots & \ddots & \vdots \\ B^{(n,1)} & B^{(n,2)} & \dots & B^{(n,n)} \end{pmatrix}, \quad (A6)$$

where each of ordered collections  $\langle B^{(i,1)}, \dots, B^{(i,n)} \rangle$ ,  $i = 1, \dots, n$  is obtained by the permutation  $\mathbf{P} \in \mathbb{P}_n$  of the collection  $\langle A^{(1)}, \dots, A^{(n)} \rangle$  and  $\mathbb{P}_n$  is the permutation group of the  $n$ -th order. Then, the maximal eigenvalue of the matrix  $A$  coincides with the maximal eigenvalue of the  $n \times n$ -matrix  $B = A^{(1)} + \dots + A^{(n)}$ .

□ The matrix  $A$  has nonnegative elements. Therefore, according to the Frobenius theorem, its eigenvalue  $\lambda(A)$  being maximal on the absolute value is positive. Let  $\mathbf{a} \in \mathbb{R}^{nm}$ ,  $\mathbf{a} = \langle a_1, \dots, a_{nm} \rangle$  be the eigenvector which corresponds to this eigenvalue where  $a_i \geq 0$ ,  $i = 1 \div nm$ ,  $A\mathbf{a} = \lambda(A)\mathbf{a}$ . It means that

$$\sum_{j=1}^{nm} A_{ij}a_j = \lambda(A)a_i, \quad i = 1 \div nm.$$

We define the vector  $\mathbf{c} \in \mathbb{R}^m$ ,  $\mathbf{c} = \langle c_1, \dots, c_m \rangle$ ,  $c_j \geq 0$ ,  $j = 1 \div m$  where

$$c_k = \max\{a_{k+sm}; s = 0, \dots, n-1\}, \quad k = 1 \div m.$$

Then, changing  $i = k + pm$ ,  $j = l + sm$ ,  $s, p = 0, 1, \dots, n-1$ , we have

$$\lambda(A)a_{k+pm} = \sum_{s=0}^{n-1} \sum_{l=1}^m A_{k+pm, l+sm}a_{l+sm} \leq \sum_{l=1}^m \left( \sum_{s=0}^{n-1} A_{k+pm, l+sm} \right) c_l.$$

Calculating the maximum on  $p = 0, 1, \dots, n-1$  of both sides of the inequality, we obtain

$$\lambda(A)c_k \leq \sum_{l=1}^m B_{kl}c_l$$

where

$$B_{kl} = \max \left\{ \sum_{s=0}^{n-1} A_{k+pm, l+sm}; p = 0, 1, \dots, n-1 \right\} \quad (A7)$$

are matrix elements of  $B = A^{(1)} + \dots + A^{(n)}$ . This formula follows from the equality

$$\sum_{s=0}^{n-1} A_{k+pm, l+sm} = \sum_{s=0}^{n-1} \left( A^{(P(s+1))} \right)_{kl}$$

where the permutation  $P \in \mathbb{P}_n$  is defined by the number  $p$  being the line number in the block matrix (A6). Having changed the summation variable as follows  $P(s+1) \Rightarrow s$ , we find that the last expression is equal to

$$\sum_{s=0}^{n-1} \left( A^{(P(s+1))} \right)_{kl} = \sum_{s=1}^n A_{kl}^{(s)} = B_{kl}$$

and the sum in (A4) does not depend on  $p$ .

Applying the statement of Theorem I to the matrix  $A$ , in a result, we obtain the inequality  $\lambda(B) \geq \lambda(A)$ . On the other side, we take the eigenvector  $\mathbf{b}$  of the matrix  $B$  with nonnegative components that corresponds to the eigenvalue  $\lambda(B)$ . Further, we define the vector  $\mathbf{c}' = \underbrace{\langle \mathbf{b}, \mathbf{b}, \dots, \mathbf{b} \rangle}_n$ . For this vector, we have

$$A\mathbf{c}' = \langle B\mathbf{b}, B\mathbf{b}, \dots, B\mathbf{b} \rangle = \lambda(B)\mathbf{c}'.$$

Then,  $\lambda(B)$  is the eigenvalue of the matrix  $A$  with the eigenvector  $\mathbf{c}'$ . According to the definition of eigenvalue  $\lambda(A)$ , we have  $\lambda(A) \geq \lambda(B)$ . From two obtained inequalities, it follows that  $\lambda(A) = \lambda(B)$ . ■